FLUORESCENCE AND ULTRAVIOLET ABSORPTION SPECTRA AND RING-TWISTING POTENTIAL ENERGY FUNCTIONS OF 1,2-DIHYDRONAPHTHALENE IN ITS S_0 AND S_1 STATES

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The fluorescence excitation spectra (FES), dispersed fluorescence (SVLF) spectra, and ultraviolet absorption spectra of 1,2-dihydronaphthalene have been collected and analyzed. The $S_1(\pi,\pi^*)$ electronic band origin is at 34,096 cm⁻¹. The FES for the jet-cooled molecules shows the four lowest frequency vibrations in the S_1 state to be at 107, 122, 197, and 293 cm⁻¹; while the SVLF from several excitation bands shows these to be at 131, 149, 267 and 347 cm⁻¹ in the S_0 state. For both states almost all of the transition frequencies below 800 cm⁻¹ can be assigned as combinations of these low-frequency modes. The series of bands beginning with 131 cm⁻¹ for S_0 and 122 cm⁻¹ for S_1 were analyzed to determine the ring-twisting potential energy functions. For the S_0 state the barrier of about 1300 cm⁻¹ is somewhat higher than that (1132 cm⁻¹) for the analogous molecule 1,3-cyclohexadiene. For the S_1 state the barrier increases significantly.